Interactions and Disorder in Quantum Dots: Instabilities and Phase Transitions

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Using a fermionic renormalization group approach we analyse a model where the electrons diffusing on a quantum dot interact via Fermi-liquid interactions. Describing the single-particle states by Random Matrix Theory, we find that interactions can induce phase transitions (or crossovers for finite systems) to regimes where fluctuations and collective effects dominate at low energies. Implications for experiments and numerical work on quantum dots are discussed.

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A variety of finite many-body physical systems are so complex that one can only approach them statistically. Random Matrix Theory (RMT) [1] has emerged as a unifying language to describe nucleii, atoms, and molecules [2] at intermediate energies. In these systems, the low-energy physics is well described in terms of singleparticle levels forming shells, but many-body states at high enough excitation energy are randomized by interactions [3], and well described by RMT. More recently, RMT has been applied to quantum chaos and mesoscopic physics, including quantum dots [2,4]. Here, in contrast to earlier applications, RMT is a valid description of single-particle states, with the external disorder potential now inducing the randomization between these states. What happens when disorder and interactions are both present? This question is relevant to the tunnelling of electrons through realistic quantum dots, which has been the focus of much recent experimental [5.6] and theoretical [5,4,7–9] interest. In this Letter we show, using renormalization group (RG) methods, that the introduction of interactions into quantum dots can produce phase transitions (actually sharp crossovers for finite system size) in the limit of weak disorder, leading to behavior qualitatively different from the noninteracting case.

Let us focus on a two-dimensional quantum dot (QD) of linear size L. The average single-particle level spacing is Δ , the mean free path is l_{mf} , and the diffusion constant is $D = v_F l_{mf}/2$, where $v_F = k_F/m^*$ is the Fermi velocity, k_F is the Fermi momentum, m^* is the effective mass of the electron, and \hbar has been set to 1. The diffusion constant is related to another important energy scale, the Thouless energy $E_T = D/L^2$, which is the inverse of the diffusion time through the QD. When the QD is strongly coupled to leads the incoming electron's energy becomes uncertain upto E_T , and therefore the electron "samples" $g = E_T/\Delta$ single-particle states [4], leading to a tunnelling conductance of ge^2/h .

We will be interested in QDs with weak disorder $(g \gg 1)$, very weakly coupled to the leads. In this case [10] within any energy band of width E_T (the Thouless band) the energy levels are coupled by correlations described by RMT. These correlations make the energies rigid so that the probability of finding two close levels vanishes as $|\epsilon_1 - \epsilon_2|^{\beta}$. Depending on the symmetries of

the problem, there are ten universal random matrix ensembles [1,11]. We focus on the orthogonal ensemble with spin degeneracy for which $\beta=1$. Experiments [5,6] can indirectly measure the energy to add an electron to the dot (called Δ_2). For the case with spin degeneracy the distribution of Δ_2 is the sum of the distribution of single particle spacings (given approximately by the famous Wigner surmise) and a delta function at zero energy, to account for an opposite spin electron going into a singly occupied state, leading to the prediction

$$p_{RMT}(\Delta_2) = \frac{1}{2} \left[\delta(\Delta_2) + \frac{\pi}{2} \Delta_2 \exp\left(-\pi \Delta_2^2\right)\right]$$
 (1)

This distribution is bimodal and has a peak at zero energy. What is observed in experiments [5,6] has no bimodality, and looks more like a symmetric gaussian around some nonzero average. These features are also observed in numerics [5,7,8] which makes it clear that the change of shape and shift of the distribution is the result of electron-electron interactions.

The simplest extension of the noninteracting model is the constant exchange and interaction (CEI) model, where the direct interaction is modelled by a capacitive term $\hat{Q}^2/2C$, and the exchange by a $-J\vec{S}^2$ term in the Hamiltonian. The CEI model (or "universal Hamiltonian" [9,12,13] H_U) is a very natural starting point in the $g \to \infty$ limit. Using H_U does improve comparison with experiments [14], but the bimodality remains at very low temperatures. This does not agree with numerics which are carried out at T=0 and do not show bimodality.

Motivated by these questions, we have carried out a systematic study of how interactions affect low-energy properties in a disordered QD. We use a fermionic RG method developed by one of us [15], based on the formalism of Shankar [16], in which one integrates out high-energy states and looks at the flow of couplings in the low-energy theory. A divergent flow signals a transition to a phase whose low-energy physics is not perturbatively connected to the noninteracting limit. For a finite QD the phase transition will be replaced by a sharp crossover. The advantage of RG over perturbative methods is that the presence of regimes of qualitatively different low-energy behavior is made manifest.

We will assume that the interactions are strong compared to the disorder. The renormalization of the in-

teractions proceeds as in the clean limit [16], leading to a Fermi liquid (FL) theory near the Fermi surface. For spinless fermions the FL is characterized by a single-particle energy $\epsilon_0(\vec{k}) \approx v_F |\vec{k} - \vec{k}_F|$, and an interaction function $f(\vec{k}, \vec{k}')$ which parameterizes how the energy of a quasiparticle (QP) of momentum \vec{k} depends on the occupation of other QPs

$$\epsilon(\vec{k}) = \epsilon_0(\vec{k}) + \sum_{\vec{k}'} f(\vec{k}, \vec{k}') \delta n(\vec{k}')$$
 (2)

with $\delta n(\vec{k})$ denoting the change of occupation of state \vec{k} with respect to the filled Fermi sea, which is the ground state. The low-energy effective FL Hamiltonian is

$$H_{FL} = \sum_{\vec{k}} \epsilon_0(\vec{k}) \hat{n}(\vec{k}) + \frac{1}{2} \sum_{\vec{k}\vec{k}'} f(\vec{k}, \vec{k}') : \hat{n}(\vec{k}) \hat{n}(\vec{k}') :$$
(3)

where $\hat{n}(\vec{k}) = c^{\dagger}(\vec{k})c(\vec{k})$, and the creation and annihilation operators obey canonical anticommutation relations. We will focus on the Thouless band centered on the Fermi surface. In particular, there are g momentum states in this band which are completely and randomly mixed [10] to produce the eigenstates of the single-particle Hamiltonian (including disorder) $\phi_{\alpha}(\vec{k})$, with energies ϵ_{α} . In terms of these states the disordered FL Hamiltonian is

$$H_{DFL} = \sum \epsilon_{\alpha} \psi_{\alpha}^{\dagger} \psi_{\alpha} + \frac{1}{2} \sum V_{\alpha\beta\gamma\delta} \psi_{\alpha}^{\dagger} \psi_{\beta}^{\dagger} \psi_{\gamma} \psi_{\delta}$$
 (4)

We de-dimensionalize the FL interaction by $f(\vec{k}, \vec{k}') = E_T u(\theta, \theta')/g$. Note that u depends only on the angular position. One resolves the interaction into Fourier components

$$u(\theta, \theta') = u(\theta - \theta') = u_0 + \sum_{m=1}^{\infty} u_m \cos(m(\theta - \theta')) \quad (5)$$

We will be interested in the case with spin rotation invariance, where there are two FL functions, f_s for the singlet channel, and f_t for the triplet channel. The corresponding (anti)symmetrized matrix elements are

$$V_{\alpha\beta\gamma\delta}^{(s,t)} = \frac{\Delta}{4} \sum_{\vec{k},\vec{k}'} u_{s,t}(\theta,\theta') (\phi_{\alpha}^*(\vec{k})\phi_{\beta}^*(\vec{k}') \pm \phi_{\alpha}^*(\vec{k}')\phi_{\beta}^*(\vec{k}))$$
$$(\phi_{\delta}(\vec{k})\phi_{\gamma}(\vec{k}') \pm \phi_{\delta}(\vec{k}')\phi_{\gamma}(\vec{k})) \tag{6}$$

where the + sign is to be taken with the singlet and the – with the triplet. Parameterizing the FL interaction as [18] $f(\vec{k}, \vec{k}', \vec{\sigma}, \vec{\sigma}') = \Phi(\vec{k}, \vec{k}') + \vec{\sigma} \cdot \vec{\sigma}' Z(\vec{k}, \vec{k}')$, where the spin of the electron is $\vec{S} = \frac{1}{2}\vec{\sigma}$, the singlet and triplet interactions can be expressed [18] as $u_s = \Phi - 3Z$ and $u_t = \Phi + Z$.

In RMT, wavefunctions at different energies are uncorrelated (except for orthogonality). Denoting an ensemble average by <> we have, for the orthogonal ensemble

$$<\phi_{\alpha}^{*}(\vec{k})\phi_{\beta}(\vec{k}')> = <\phi_{\alpha}(-\vec{k})\phi_{\beta}(\vec{k}')> = \frac{\delta_{\alpha\beta}\delta_{\vec{k}\vec{k}'}}{a}$$
 (7)

The only matrix elements with nonzero average are $\langle V_{\alpha\beta\beta\alpha}^{(s)} \rangle = u_{s0}\Delta$, $\langle V_{\alpha\beta\beta\alpha}^{(t)} \rangle = u_{t0}\Delta$, and $\langle V_{\alpha\alpha\beta\beta}^{(s)} \rangle = u_{s}(\pi)\Delta/g$. The first two terms when rearranged produce the CEI model [9], while the last term is a Cooper interaction, which however, is suppressed for our Fermi liquid by 1/g. Since g is assumed large we ignore it henceforth [9].

One can similarly calculate the variances of the matrix elements. Here one has to pay attention to the subtle correlations between different eigenfunctions induced by orthogonality [1]. One finds that u_{s0} and u_{t0} produce no fluctuations. The general expression is

$$\langle V_{\alpha\beta\gamma\delta}^2 \rangle - \langle V_{\alpha\beta\gamma\delta} \rangle^2 = \frac{\Delta^2}{4g^2} \sum_{m=1}^{\infty} u_m^2$$
 (8)

Kurland et al argued [12] that since these fluctuations vanish in the limit $g \to \infty$ the universal Hamiltonian is exact in this limit. On the other hand, because of their large number, fluctuation terms can have important effects [17]. The best way to see whether the fluctuation terms are important for low-energy physics (such as the conductance peak spacing experiments) is to carry out an RG analysis and see how these terms scale. If interactions beyond the universal Hamiltonian grow, they will dominate the low-energy physics no matter how weak they are in the microscopic Hamiltonian.

We begin with g states in the Thouless band around the Fermi surface. We successively integrate out single-particle states farthest from the Fermi surface, and at some stage in the procedure we have g' states. We will define the flow parameter l of the RG by $g'(l) = ge^{-l}$ (with $\frac{d}{dl} = -g'\frac{d}{dg'}$). We do not rescale the energy, since that would also rescale Δ , which we want to retain as a physical parameter. We want to integrate out the states at $\pm g'/2$ to 1-loop order. However, all 1-loop diagrams have two internal lines. One of these lines is the state at $\pm g'/2$. The other should be summed over all lower energy states $|g''| \leq |g'|/2$. This abolishes all reference to the states g'/2 and higher in the effective theory. Each set of internal lines contributes the following change to the interaction matrix elements

$$\frac{dV_{\alpha\beta\gamma\delta}^{(s)}}{dl} = -\frac{g'}{2}G_1(\mu,\nu)V_{\alpha\beta\mu\nu}^{(s)}V_{\nu\mu\gamma\delta}^{(s)} + g'G_2(\mu,\nu) \times \left(V_{\alpha\mu\nu\gamma}^{(s)}V_{\beta\nu\mu\delta}^{(s)} - \frac{3}{4}V_{\alpha\mu\nu\gamma}^{(s+t)}V_{\beta\nu\mu\delta}^{(s+t)} + (\alpha \leftrightarrow \beta)\right)$$

$$\frac{dV_{\alpha\beta\gamma\delta}^{(t)}}{dl} = -\frac{g'}{2}G_1(\mu,\nu)V_{\alpha\beta\mu\nu}^{(t)}V_{\nu\mu\gamma\delta}^{(t)} + g'G_2(\mu,\nu)$$

$$\left(V_{\alpha\mu\nu\gamma}^{(t)}V_{\beta\nu\mu\delta}^{(t)} + \frac{1}{4}V_{\alpha\mu\nu\gamma}^{(s+t)}V_{\beta\nu\mu\delta}^{(s+t)} - (\alpha \leftrightarrow \beta)\right) \tag{9}$$

where
$$V^{(s+t)} = V^{(s)} + V^{(t)}$$
, $G_1(\mu, \nu) = (1 - n_{F\mu} - n_{F\nu})/(\epsilon_{\mu} + \epsilon_{\nu})$ and $G_2(\mu, \nu) = (n_{F\nu} - n_{F\mu})/(\epsilon_{\mu} - \epsilon_{\nu})$.

In order to make further analytical progress we ensemble average the internal lines of the diagram (μ, ν) . The rationale is that in the course of integrating out states we will have to sum over many many states (μ, ν) . In order to carry out the average we use

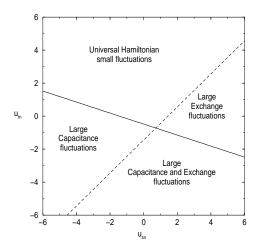


FIG. 1. Phase diagram in the $g \to \infty$ limit. Four different phases emerge.

$$<\phi_{\mu}^{*}(1)\phi_{\mu}(2)\phi_{\nu}^{*}(3)\phi_{\nu}(4)> = \frac{\delta_{12}\delta_{34}}{g^{2}} - \frac{\delta_{1,-3}\delta_{2,-4} + \delta_{14}\delta_{23}}{g^{3}}$$

$$(10)$$

At any stage in the RG it is g, and not g', that appears in these averages, since at one-loop there is no wavefunction renormalization, and the original wavefunction correlations remain unchanged. With this averaging, the change in interaction matrix elements can be absorbed into a change in the FL parameters. The resulting flow equations to zeroth order in 1/g (for $n \neq 0$) are

$$\frac{du_{sn}(l)}{dl} = Ce^{-l} \left((u_{sn}(l))^2 - \frac{3}{4} (u_{sn}(l) + u_{tn}(l))^2 \right)$$

$$\frac{du_{tn}(l)}{dl} = -Ce^{-l} \left((u_{tn}(l))^2 + \frac{1}{4} (u_{sn}(l) + u_{tn}(l))^2 \right) \quad (11)$$

where $C = \log{(2)}$ comes from the integration over energies less than g'. Each moment n of the Fermi liquid function is not mixed with any other moment n', and u_{s0} , u_{t0} do not flow. The flow equations have an explicit dependence on the flow parameter l, but this dependence can be removed by defining a new coupling $\tilde{u}_n(l) = e^{-l}u_n(l)$, which are the FL parameters for a "rescaled" QD with a rescaled Thouless energy $E'_T = e^{-l}E_T$ (corresponding to $g' = e^{-l}g$ completely randomized states). Rewriting the above equations in terms of $\tilde{\Phi}_n = (\tilde{u}_{sn} + 3\tilde{u}_{tn})/4$ and $\tilde{Z}_n = (\tilde{u}_{tn} - \tilde{u}_{sn})/4$ we obtain

$$\frac{d\tilde{\Phi}_n(l)}{dl} = -\tilde{\Phi}_n - 2C\tilde{\Phi}_n^2$$

$$\frac{d\tilde{Z}_n(l)}{dl} = -\tilde{Z}_n - 2C\tilde{Z}_n^2$$
(12)

The decoupling of $\tilde{\Phi}_n$ and \tilde{Z}_n is a consequence of spin rotation invariance. From these flow equations we now construct the phase diagram that is the central result of our paper. Clearly, there are unstable fixed points at $\tilde{\Phi}_n = -1/2C$ and $\tilde{Z}_n = -1/2C$ which separate weak and strong coupling phases. There are four phases (Figure 1): (i) A phase where both Φ_n and Z_n have small fluctuations, whose low-energy physics is controlled by the

universal Hamiltonian. (ii) A phase where Z_n diverges but Φ_n remains small, in which the capacitance will have small fluctuations but the exchange interaction will acquire large fluctuations. (iii) A phase where Φ_n diverges but Z_n remains small, in which there are large capacitance fluctuations, but the exchange energy has small fluctuations. (iv) Finally, a phase in which both Φ_n and Z_n flow to strong coupling.

The same flow equations and phase diagram are obtained in the unitary case if time-reversal symmetry is broken by the coupling of an applied magnetic field to the orbital sector only, as happens in GaAs dots.

Let us consider the implications for a real quantum dot. Here $g \approx 10-100$ is typical, which is not particularly large. This means that the RG flow should be stopped when $g'=ge^{-l}\approx 1$. In the strongly fluctuating phases the fluctuations will increase, but the flow will be cutoff at the nonuniversal scale $l^*\approx \log{(g)}$ and the putative phase transition will be replaced by a crossover. Nevertheless, we can expect that fluctuations of the matrix elements play an important role at low energies.

The peak spacing distribution can be qualitatively understood by a two-level example, considered by Levit and Orgad [8]. The resulting peak spacing distribution is approximately gaussian with a mean position controlled by the constant interaction (which is u_{s0} , u_{t0} in our language), and a variance given approximately by [8]

$$<\Delta_2^2> = 4\left[- < V_{1221}>^2\right] + \frac{4\Delta^2}{\pi}$$
 (13)

If bare interaction matrix elements are used in the above equation, their contribution is down by $1/g^2$ compared to the single-particle contribution and negligible (assuming that $|u_n(l=0)| \ll g$). In the regime of weak fluctuations this remains true, and the width of the distribution is controlled mainly by single-particle effects. However, it is clear that in the regime of strong fluctuations the variance of the interaction matrix elements can dominate the single-particle contribution, and thus the width of this distribution should increase with interaction strength, as has been observed in numerical work [5,7,8].

The flow equations also have implications for interaction effects on the width of the quasiparticle levels [19]. Based on bare matrix elements, the prediction is that quasiparticle peaks should be relatively well-defined for energies $\epsilon \leq \Delta \sqrt{g}$, while they acquire a width larger than the single particle spacing at larger energies. If one is well into a strongly fluctuating phase, one expects that this threshold energy is pushed down and may even become zero. In this case the system would not be a Fermi liquid and the conductance peaks will have a finite width even at T=0 (which has been seen experimentally [20]).

Consider now FL instabilities. In the clean system, the FL becomes unstable whenever any of the Φ_n , $Z_n \leq -1$ [18]. In the two-level example, the energy to add a particle is controlled by $V_{\alpha\beta\beta\alpha}$ where one of the levels is occupied and the other empty. In turn this matrix element is

the sum of its average (controlled by u_{s0} , u_{t0}) and a fluctuation part (controlled by u_{sn} , u_{tn}). If the fluctuations overpower the constant interaction, this matrix element can become negative, leading to a "bunching" instability [21,22] in which more than one particle can be added to the QD. The charge/spin density wave instability of the clean system when Φ_n , $Z_n \leq -1$ will be modified by disorder and finite-size effects. The characterization of such a ground state is an open problem.

Our approach can be easily generalized to other ensembles [1,11] and the results will be reported in forthcoming work. It is tempting to speculate about the connection with a putative metal-insulator transition in an infinite two-dimensional system [23,24]. However, our analysis is limited to the zero-dimensional case. Strong fluctuations in the matrix elements would have implications for the distribution of persistent currents in mesoscopic structures [25]. Also relevant is the effect of a weak magnetic field, which enhances fluctuations [26], on the phase diagram. Finally, for realistic QD's, corrections to universal RMT behavior (of order 1/g) [4] may be important.

In closing, RMT is a rich field with applications to nucleii, atoms and molecules, where interactions randomize excited states [3]. We have shown that in QD's interactions and disorder can combine to produce a state in which fluctuations in interaction matrix elements become large, in which quasiparticles may cease to be well-defined at arbitrarily low energies, and the behavior is dominated by collective effects.

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